# International Journal of Quantum Chemistry Author Index—Volume 66


**Amovilli, C.**
—; March, N. H.: Kinetic Energy Density in Terms of Electron Density for Closed-Shell Atoms in a Bare Coulomb Field, 281

**Andrés, J.**
—; Domingo, L. R.; Picher, M. T.; Safont, V. S.: Comparative Theoretical Study of Transition Structures, Barrier Heights, and Reaction Energies for the Intramolecular Tautomerization in Acetaldehyde/Vinyl Alcohol and Acetaldimine/ Vinylamine Systems, 9

**Arakane, F.**
—; Matsuoka, O.: Recurrence Formulas for Molecular Integrals over Laguerre Gaussian-Type Functions, 273

**Arimoto, S.** See Mezey, P. G., 99

**Baumgarten, M.** See Tyutyulkov, N., 425

**Bauschlicher, C. W., Jr.**
QCISD(T) and B3LYP Can Correctly Describe the EA of B, Al, and Ga, 285

**Béccar Varela, M. P.** See Ferraro, M. B., 31

**Bendazzoli, G. L.**
—; Evangelisti, S.: Asymptotic Behavior of the RHF Energy of the PPP Model of Alternant Cyclic Polyenes, 397

**Brändas, E. J.**
Review of *Molecular Physics and Elements of Quantum Chemistry: Introduction to Experiments and Theory*, by H. Haken and H. C. Wolf, 109
Review of *The Physics of Atoms and Quanta: Introduction to Experiments and Theory*, by H. Haken and H. C. Wolf, 109

**Burton, P. J.**
—; Gould, M. D.: Matrix Elements of $U(2n)$ Generators in a Multishell Spin–Orbit Basis. I. The Del-Operator MEs in a Two-Shell Composite Gelfand–Paldus Basis, 323
—; Gould, M. D.: Matrix Elements of $U(2n)$ Generators in a Multishell Spin-Orbit Basis. II. The Two-Shell Nonzero Shift ACCs and $U(2n)$ Generator MEs, 345
—; Gould, M. D.: Matrix Elements of $U(2n)$ Generators in a Multishell Spin-Orbit Basis. III. General Formulas, 365

**Büsse, G.**
—; Kleindienst, H.; Lüchow, A.: Nonrelativistic Energies for the Be Atom: Double-linked Hylleraas–CI Calculation, 241

**Canuto, S.** See Coutinho, K., 249

**Cao, Z.**
—; Wu, W.; Zhang, Q.: Construction and Applications of Symmetrized Valence Bond Wave Functions, 1

**Caputo, M. C.** See Ferraro, M. B., 31

**Cardelino, B. H.**
—; Moore, C. E.; Frazier, D. O.; Musaev, D. G.; Morokuma, K.: Ab Initio Calculations on the Diacetylene Dimer: HCCCC(H)C(H)CCCH, 189

**Cheng, W.** See Tang, A. C., 113

**Coutinho, K.**
—; De Oliveira, M. J.; Canuto, S.: Sampling Configurations in Monte Carlo Simulations for Quantum Mechanical Studies of Solvent Effects, 249

**De Oliveira, M. J.** See Coutinho, K., 249

**Diaz, C. G.** See Radicioni, M. D., 261

**Dietz, F.** See Tyutyulkov, N., 425

**Domingo, L. R.** See Andrés, J., 9

**Edvardsson, D.** See Fängström, T., 203

**Enkvist, C.** See Fängström, T., 203

**Ericsson, M.** See Fängström, T., 203

**Evangelisti, S.** See Bendazzoli, G. L., 397

**Fängström, T.**
—; Edvardsson, D.; Ericsson, M.; Lunell, S.; Enkvist, C.: Density Functional Study of Chlorine–Oxygen Compounds Related to the ClO Self-Reaction, 203

**Fernández, F. M.** See Radicioni, M. D., 261

**Ferraro, M. B.**
—; Caputo, M. C.; Béccar Varela, M. P.; Lazzeretti, P.: Calculation of Magnetic Properties of HF, $H_2O$, $NH_3$, and $CH_4$ Molecules Using a Longitudinal Gauge for the Vector Potential, 31

**Flores-Riveros, A.**
Generalized Hylleraas–Gaussian Basis Sets Applied to the Variational Treatment of Two-Electron Atoms, 287
—; See Ley-Koo, E., 123

**Frazier, D. O.** See Cardelino, B. H., 189

**Fukui, K.** See Mezey, P. G., 99

**Fulde, P.** See Kladko, K., 377

**Gopi Mohan, C.**
—; Mishra, P. C.: Electrostatic Potential Mapping Using Hybridization Displacement Charge: Atomic Parameters and Transferability of Charge and Potential, 149

**Gould, M. D.** See Burton, P. J., 323, 345, 365
**Green, A. E. S.**
—; Zanardi, M.: Cellulose Pyrolysis and Quantum Chemistry, 219
**Gregory, F.**
Review of *The Conscious Mind: In Search of a Fundamental Theory*, by David J. Chalmers, 107

**Hamed, M. M.** See Mohamed, A. A., 415
**Han, Y. K.** See Kim, Y. S., 91
**Hilger, R.**
—; Merckens, H.-P.; Lüchow, A.; Kleindienst, H.: Upper- and Lower-Bound Hylleraas–CI Calculations for the Nonrelativistic $P^o$ States of the $^4$He Isotope, 25
**Hirao, K.** See Nakayama, K., 157

**Järv, J.** See Sak, K., 391
**Jursic, B. S.**
Complete Basis Set Ab Initio and Hybrid Density Functional Theory Exploration of the Potential Energy Surface in the Reaction Between an Amino Radical and Nitrogen Oxide, 409

**Karelson, M.** See Sak, K., 391
**Kendrick, B.**
Erratum: The Effects of Pseudomagnetic Fields in Molecular Spectra and Scattering, 111
**Kim, Y. S.**
—; Lee, S. Y.; Oh, W. S.; Park, B. H.; Han, Y. K.; Park, S. J.; Lee, Y. S.: Karmers' Unrestricted Hartree–Fock and Second-Order Møller–Plesset Perturbation Methods Using Relativistic Effective Core Potentials with Spin–Orbit Operators: Test Calculations for HI and $CH_3I$, 91
**Kladko, K.**
—; Fulde, P.: On the Properties of Cumulant Expansions, 377
**Kleindienst, H.** See Hilger, R., 25
—; See Büsse, G., 241
**Kovalenko, A.**
Extended States of the Shallow Donor Located near a Semiconductor–Insulator Interface, 435
**Kovarsky, V. A.**
Multiquantum Processes in the Enzyme Molecules Immobilized on Biological Membranes, 255

**Lagowski, J. B.** See Subramanian, H., 229
**Lazzeretti, P.** See Ferraro, M. B., 31
**Lee, S. Y.** See Kim, Y. S., 91
**Lee, Y. S.** See Kim, Y. S., 91
**Ley-Koo, E.**
—; Flores-Flores, A.: Helium Atom Inside Boxes with Paraboloidal Walls, 123
**Li, Q. S.** See Tang, A. C., 113
**Lüchow, A.** See Hilger, R., 25
See Büsse, G., 241
**Lunell, S.** See Fängström, T., 203
**Luzzi, R.** See Mesquita, M. V., 177

**Madjarova, G.** See Tyutyulkov, N., 425
**Manoharan, M.**
—; Venuvanalingam, P.: Theoretical Investigation on the Reactivity of Sulfur-Centered Heterocumulenes as Dienophiles in Diels–Alder Reactions and Endo-Lone-Pair Effect, 309
**March, N. H.** See Amovilli, C., 281
**Matsuoka, O.** See Arakane, F., 273
**Meng, Q. B.** See Wu, Z. J., 301
**Merckens, H.-P.** See Hilger, R., 25
**Mesquita, M. V.**
—; Vasconcellos, Á. R.; Luzzi, R.: Positive-Feedback-Enhanced Fröhlich's Bose–Einstein-Like Condensation in Biosystems, 177
**Mezey, P. G.**
—; Fukui, K.; Arimoto, S.; Taylor, K.: Polyhedral Shapes of Functional Group Distributions in Biomolecules and Related Similarity Measures, 99
**Mishra, P. C.** See Gopi Mohan, C., 149
**Mohamed, A. A.**
—; Hamed, M. M.: Electronic Spectra of Phenyl-, 3-Pyridyl-Furfuryl-, and 2-Theinyl-Imino Derivatives of Thiazole: Molecular Orbital Treatment, 415
**Moore, C. E.** See Cardelino, B. H., 189
**Morley, J. O.**
Theoretical Studies on the Structure and Electronic Properties of Aryl Sulfides and Sulfones, 141
**Morokuma, K.** See Cardelino, B. H., 189
**Musaev, D. G.** See Cardelino, B. H., 189

**Nakano, H.** See Nakayama, K., 157
**Nakayama, K.**
—; Nakano, H.; Hirao, K.: Theoretical Study of the $\pi \rightarrow \pi^*$ Excited States of Linear Polyenes: The Energy Gap Between $1^1B_u^-$ and $2^1A_g^-$ States and Their Character, 157

**Oh, W. S.** See Kim, Y. S., 91

**Park, B. H.** See Kim, Y. S., 91
**Park, S. J.** See Kim, Y. S., 91
**Picher, M. T.** See Andrés, J., 9
**Pyykkö, P.** See Runeberg, N., 131

**Radicioni, M. D.**
—; Diaz, C. G.; Fernández, F. M.: Renormalized Perturbation Theory by the Moment Method for Degenerate States: Anharmonic Oscillators, 261
**Runeberg, N.**
—; Pyykkö, P.: Relativistic Pseudopotential Calculations on $Xe_2$, RnXe, and $Rn_2$: The van der Waals Properties of Radon, 131

**Safont, V. S.** See Andrés, J., 9
**Sak, K.**
—; Karelson, M.; Järv, J.: Quantum Chemical Modelling of the Effect of Proline Residues on Peptide Conformation, 391
**Starikov, E. B.**
A Comparative Three-Dimensional Hartree–Fock Crystal

Orbital Study of Double-Stack Organic Charge-Transfer (Semi)conductors: TTF–TCNQ, TTF–DCNQI, and TTF–2,5-$Me_2$-DCNQI, 47

Ab Initio Hartree–Fock Crystal Orbital Studies on Charge-Transfer Complexes: Different Crystal Modifications of the Same Compounds, 69

**Subramanian, H.**

—; Lagowski, J. B.: Trends in Geometric and Electronic Properties of Thiophene- and Cyclopentadiene-Based Polymers, 229

**Tang, A. C.**

—; Li, Q. S.; Cheng, W.: Vibrational Spectra of Icosahedral ($I_h$ and $I$) Fullerenes, 113

**Taylor, K.** See Mezey, P. G., 99

**Tyutyulkov, N.**

—; Madjarova, G.; Dietz, F.; Baumgarten, M.: Organic Polymers with Indirect Magnetic Interaction Caused by the Symmetry of the Elementary Units, 425

**Vasconcellos, Á. R.** See Mesquita, M. V., 177

**Venuvanalingam, P.** See Manoharan, M., 309

**Wu, W.** See Cao, Z., 1

**Wu, Z. J.**

—; Meng, Q. B.; Zhang, S. Y.: Theoretical Investigation of $LaC_3^{n+}$ ($n$ = 0, 1, 2) Clusters by Density Functional Theory, 301

**Xie, D.**

—; Yan, G.: A Theoretical Procedure for Determining Rovibrational Eigenstates of van der Waals Complexes, 119

**Yan, G.** See Xie, D., 119

**Zanardi, M.** See Green, A. E. S., 219

**Zhang, Q.** See Cao, Z., 1

**Zhang, S. Y.** See Wu, Z. J., 301

# International Journal of Quantum Chemistry Subject Index—Volume 66


Ab initio molecular orbital theory, 229
Ab initio, 69, 189
AM1, 309
Anharmonic oscillator, 261
Ar—HCl complex, 119
Aryl sulfides, 141
Asymptotic behavior, 397
Asynchronous process, 9

Bare Coulomb field, 281
Basis set ab initio, 409
Be atom, 241
Biological membrane, 255
Biomass energy, 219
Biomolecules, 99
Biosystems, 177
B3LYP, 285

C8H4, 189
Cellulose pyrolysis, 219
Cellulose, 219
Charge-transfer complexes, 47, 69
Chemical bonds, 1
Chlorine–Oxygen Compounds, 203
ClO Self-Reaction, 203
Comparison of several calculation methods, 9
Conducting polymers, 229
Configuration interaction, 119
Coupled cluster approach, 285
CRYSTAL 92 Routine Package, 69
Crystal orbital, 69
Cumulants, 377
Cyclic polienes, 397

Degenerate states, 261
Del-Operator MEs, 323
Density functional theory, 409
Density functional theory (DFT), 189, 203, 281, 301
Diacetylene, 189
Diels–Alder reaction, 309
Dimer, 189
Diphenyl sulfide, 141
Double-linked basis set, 241

Electronic structure, 123
Enzyme processes, 255
Exchange energy, 397
Excited states, 157
Excited-state energy gaps, 157
Explicitly correlated wave function, 241
Extended electronic states, 435

Finite size correction, 397
Fröhlich effect, 177
Functional group, 99

Gauge invariance, 31
Gaussian 92/DFT, 301
Gaussian-type function, 273
Gelfand–Paldus basis, 323
Geometry optimization, 415
Ground-state electron density, 281
Ground-state energy, 241
Group character, 113

Hartree–Fock, 69
Hartree–Fock crystal orbital approximation, 47
Helium atom, 123
Hybridization displacement charge, 149
Hylleraas–CI, 25, 241
Hylleraas–Gaussian basis sets, 287

Icosahedral fullerenes, 113
Icosahedral group, 113
Immobilized enzyme, 255
Indirect magnetic interaction, 425
INDO/S-CI, 415
Infrared spectra, 113
Intramolecular hydrogen shift, 9

Keto/enol and imine/enamine tautomerizations, 9
Kinetic energy density, 281
Kramers' restricted Hartree–Fock (KRHF), 91

$LaC_3^{n+}$, 301
Laguerre, 273

Macroscopic properties, 377
Magnetic shielding tensor, 31
Magnetic susceptibility, 31
Many-electron systems, 323
Matrix elements, 323, 345, 365
MO calculations, 415
Model of atoms trapped inside solids, 123
Molecular integral, 273
Molecular orbital calculations, 141
Moment method, 261
Monte Carlo simulations, 249
MRMP, 157
Multireference-based perturbation theory, 157
Multishell spin–orbit basis, 323, 345, 365
Multistage decay scheme, 219

Nontrivial geometry, 377

Organic crystals, 47
Oxidation–reduction reaction, 255

Pariser–Parr–Pople, 397
Peptide conformation, 391
Perturbation theory, 25
Photoionization cross section, 435
PM3, 309
Polar vibrations, 177
Polarizability of trapped atoms, 123
Polycyclopentadiene, 229
Polyenes, 157
Polyfulvene, 229
Polyhedral models, 99
Polymers, 425
Polythiophene, 229
Potential energy surface, 409
Pressure, 123
Projection operator, 1
Proline residues, 391

Pseudopotentials, 131
*P* states of $^4$He, 25

QCISD(T), 285
Quadrupole moment, 123

Radon, 131
Raman spectra, 113
Recurrence formula, 273
Relativistic effective core potentials (RECP), 91
Relativistic effects, 131
Renormalized perturbation theory, 261
Rovibrational eigenstates, 119

Scattering, 435
Second-order Møller–Plesset perturbation (KRMP2), 91
Self-consistent field, 119
Semi-empirical molecular orbital theory (MNDO, AM1), 229
Semiconductor–insulator interface, 435
Semiempirical AM1 calculations, 391
Semiempirical method, 309
Shallow donor, 435
Solid, 377
Solvatochromism, 249
Solvent effects, 249
Sonine polynomial, 273
Spectra, 415
Spin–orbit, 131
Spin–orbit operators, 91
Structure, 301
Sulfene, 309
Sulfine, 309
Sulfones, 141
Symmetry, 1, 425

Thiazoles, 415
Tranferability of properties, 149
Transition energy, 1
Transition structures, 9, 309
Two-component spinors, 91
Two-electron atoms, 287
Two-shell nonzero shift ACCs, 345

Upper and lower bounds, 25

van der Waals complexes, 119
van der Waals radii, 131
Variance minimization, 25
VB wave function, 1
Vibrational frequency, 301